# Solute transport in a heterogeneous aquifer: a search for nonlinear deterministic dynamics

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Nonlinear Processes in Geophysics (2005) 12: 211–218
SRef-ID: 1607-7946/npg/2005-12-211
European Geosciences Union


Nonlinear Processes in Geophysics

# Solute transport in a heterogeneous aquifer: a search for nonlinear deterministic dynamics

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Part of Special Issue "Nonlinear deterministic dynamics in hydrologic systems: present activities and future challenges"

**Abstract.** The potential use of a nonlinear deterministic framework for understanding the dynamic nature of solute transport processes in subsurface formations is investigated. Time series of solute particle transport in a heterogeneous aquifer medium, simulated using an integrated probability/Markov chain (TP/MC) model, groundwater flow model, and particle transport model, are studied. The correlation dimension method, a popular nonlinear time series analysis technique, is used to identify nonlinear determinism. Sensitivity of the solute transport dynamics to the four hydrostratigraphic parameters involved in the TP/MC model: (1) number of facies; (2) volume proportions of facies; (3) mean lengths (and thereby anisotropy ratio of mean length) of facies; and (4) juxtapositional tendencies (i.e. degree of entropy) among the facies is also studied. The western San Joaquin Valley aquifer system in California is considered as a reference system. The results indicate, in general, the nonlinear deterministic nature of solute transport dynamics (dominantly governed by only a very few variables, on the order of 3), even though more complex behavior is possible under certain (extreme) hydrostratigraphic conditions. The sensitivity analysis reveals: (1) the importance of the hydrostratigraphic parameters (in particular, volume proportions of facies and mean lengths) in representing aquifer heterogeneity; and (2) the ability of the correlation dimension method in capturing the (extent of) complexity of the underlying dynamics. Verification and confirmation of the present results through use of other nonlinear deterministic techniques and assessment of their reliability for a wide range of solute transport scenarios are recommended.

## 1 Introduction

Adequate knowledge of subsurface flow and solute transport processes is crucial for effective and efficient management of our water resources and environment. As flow and transport in subsurface formations are strongly affected by the hydraulic properties of the medium, their reliable assessment requires detailed aquifer characterization. The past decades witnessed numerous models for aquifer heterogeneity, flow and transport. Most of these employ the concept of stochastic field/process (e.g. Gelhar, 1993; Dagan, 2000; Zhang, 2002), as it is generally assumed that the heterogeneous nature of aquifers results in random behaviors of flow and transport. The temporal and spatial variability exhibited by these processes may, in many cases, justify this assumption. The ability of these models to fairly represent the basic statistical properties (e.g. mean, variance) of flow and transport processes may have further strengthened our view on the usefulness of stochastic field/process concept for subsurface problems.

However, as aquifer heterogeneity and the associated flow and transport processes at some scales are not as irregular and complex as those at other scales (suggesting possible simplicity in the former), the appropriateness of the stochastic field/process concept for every subsurface problem remains unclear. This comes into further question with our knowledge of nonlinear deterministic chaos theory (Lorenz, 1963), according to which complex and irregular looking processes might also be the outcome of simple deterministic systems with only a few nonlinear interdependent variables with sensitive dependence on initial conditions.

Searching for the possible presence of nonlinear determinism in hydrologic processes and employing nonlinear deterministic techniques to predict their dynamics have been important research activities in hydrology in recent times (see Sivakumar, 2000, 2004 for reviews). The outcomes of such studies are encouraging, as they have not only revealed possible deterministic nature of hydrologic processes but also reported extremely good predictability of their evolutions. Furthermore, comparisons between hydrologic predictions using nonlinear deterministic techniques and others (e.g. stochastic methods and neural networks) have indicated better (or at least equally good) performance of the former compared to the latter (e.g. Sivakumar et al., 2002a, b).

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The above studies, however, have essentially concentrated on surface hydrologic processes (e.g. rainfall, river flow, rainfall-runoff, lake volume, and sediment transport). In spite of the encouraging results, the use of nonlinear deterministic concepts in solving subsurface problems has not received much attention. This issue is addressed in the present study, driven by the fact that, despite the complexities involved in subsurface flow and transport processes, the permanent nature of soils and aquifer types bring some kind of determinism and order to the subsurface mechanisms (Gelhar, 1993). As a first step in this direction, the study investigates the possible presence of deterministic dynamics in the solute transport processes in a heterogeneous aquifer medium. The transport process is simulated by integrating a transition probability/Markov chain (TP/MC) aquifer representation model (Carle and Fogg, 1996) with a groundwater flow (MODFLOW) model (Harbaugh et al., 2000) and a random walk particle transport (RWHet) model (LaBolle et al., 1996). The correlation dimension method (Grassberger and Procaccia, 1983) is employed to identify determinism.

The TP/MC approach incorporates "soft" geologic information into Markov-chain models of spatial variability to produce geologically plausible realizations of subsurface heterogeneity. The approach describes aquifer hydrogeology in terms of its major hydrostratigraphic units (facies) rather than by extensive knowledge of the aquifer hydraulic conductivity distribution (the latter being the basis for Gaussian stochastic models). The hydrostratigraphy is characterized in a probabilistic manner by four geostatistical model parameters: (1) the number of identifiable major facies; (2) the volume proportions of facies; (3) the mean lengths (and thereby anisotropy ratio of mean length) of facies; and (4) juxtapositional tendencies (i.e. degree of entropy) among the facies. Appropriate selection of these parameters in the TP/MC model is critical for reliable aquifer heterogeneity representations, although such a selection is typically hampered by the lack of sufficient data, an issue addressed in sensitivity analysis. Therefore, a limited sensitivity analysis of these parameters with respect to the dynamic behavior of solute transport process is also investigated herein. The western San Joaquin Valley aquifer system in California (Belitz and Phillips, 1995) is considered as a reference system for this analysis.

## 2 Models for aquifer representation, flow dynamics, and solute transport

The solute transport process in Markov chain random fields is simulated by integrating a transition probabilility/Markov chain aquifer representation model, a groundwater flow model, and a random walk particle transport model. The basic mathematical concepts of these models are briefly reviewed below.

In the TP/MC model (Carle and Fogg, 1996; Carle, 1999), readily observable geologic attributes (e.g. volume proportions, mean lengths, and juxtapositional tendencies) can be incorporated directly into development of a three-dimensional Markov chain model through a combination of fitting to transition probability measurements and inference from geologic concepts and principles. The Markov chain model is then used in a conditional sequential indicator simulation and simulated quenching to generate "realizations" of subsurface facies distributions. The transition probability, $t_{jk}(\boldsymbol{h})$, is defined as the conditional probability that a geologic facies of category $k$ occurs at a spatial location $\boldsymbol{x}+\boldsymbol{h}$ given that a facies of category $j$ occurs at a location $\boldsymbol{x}$:

$$t_{jk}(\boldsymbol{h}) = Pr\,\{k \text{ occurs at } \boldsymbol{x}+\boldsymbol{h} | j \text{ occurs at } \boldsymbol{x}\}, \tag{1}$$

where $0 \le t_{jk}(\boldsymbol{h}) \le 1$, $\boldsymbol{x}$ is a spatial location vector, and $\boldsymbol{h}$ is a separation or lag distance vector. Measurements of $t_{jk}(h_\phi)$, where $\phi$ is the direction, reflect the spatial continuity and juxtapositional tendencies of the facies. Juxtapositional tendencies can be related to entropy (order/disorder) of transition probabilities of embedded occurrence. The entropy, $E_j$, of juxtapositional tendencies in a direction $\phi$ is expressed as:

$$E_{j,\phi} = -\sum_{k=1}^{K} r_{jk,\phi} \ln(r_{jk,\phi}), \tag{2}$$

where $r_{jk,\phi}=Pr$ $\{k$ is juxtaposed to $j$ in the direction $\phi|$ an embedded occurrence of $j\}$.

The groundwater flow in the heterogeneous aquifer is assumed to be subject to steady state three-dimensional saturated incompressible flow:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial \Phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial \Phi}{\partial z}\right) = 0 \text{ on } x, y, z\ \varepsilon\ \Omega, \tag{3}$$

where $K_{xx}$, $K_{yy}$, and $K_{zz}$ are hydraulic conductivities in $x$, $y$, and $z$ directions, respectively, $\Phi$ is hydraulic or piezometric head, and $\Omega$ is domain of interest. No-flow and constant head condition are specified for the boundaries of the flow domain. The flow process is simulated using the finite difference flow code MODFLOW (Harbaugh et al., 2000).

For solute transport simulation, we use a random-walk particle method (RWPM) to solve the standard advection-dispersion equation (ADE), an approach widely used for transport modeling in heterogeneous media (e.g. Tompson and Gelhar, 1990). The method used herein is a variant of the standard RWPM that provides both local and global conservation of mass (LaBolle et al., 1996). The method applies a correction to the standard advection-dispersion equation

$$\frac{\partial}{\partial t}\left[\Theta(X,t)c(X,t)\right] = -\sum_i \frac{\partial}{\partial x_i}\left[v_i(X,t)\Theta(X,t)c(X,t)\right] + \sum_{i,j}\frac{\partial}{\partial x_i}\left[\Theta(X,t)D_{ij}(X,t)\frac{\partial c(X,t)}{\partial x_j}\right] \tag{4}$$

by including an additional term, which takes care of discontinuities, and is given by:

$$\frac{\partial}{\partial t}\left[\Theta(X,t)c(X,t)\right] = -\sum_i \frac{\partial}{\partial x_i}\left[v_i(X,t)\Theta(X,t)c(X,t)\right]$$

$$+\sum_{i,j}\frac{\partial}{\partial x_i}\left[\Theta(X,t)D_{ij}(X,t)\frac{\partial c(X,t)}{\partial x_j}\right]$$
$$+\sum q_k(x,t)c_k(x,t)\delta_k(x-x_k), \tag{5}$$

where $t$ is time, $c$ is concentration, $v_i$ is pore water velocity, $\Theta$ is effective volumetric water content (or effective porosity), $c_k$ is the aqueous phase concentration in the flux $q_k$ of water at $x_k$, $D_{ij}$ is a real symmetric dispersion tensor given as

$$D_{ij}=(\alpha_T\,|v|+D'_d)\delta_{ij}+(\alpha_L-\alpha_T)v_iv_j/\,|v|\,, \tag{6}$$

where $\alpha_T$ and $\alpha_L$ are transverse and longitudinal dispersivities, respectively, and $D'_d$ is effective molecular diffusivity, $\delta_{ij}$ is the Dirac delta function. The program RWHet (Random Walk particle model for simulating transport in Heterogeneous Permeable Media) of LaBolle (2000) is used for implementing the modified RWPM.

## 3 Correlation dimension method

The correlation dimension method uses the correlation integral (or function) to identify determinism (or distinguish determinism and stochasticity). Herein, the Grassberger-Procaccia correlation dimension algorithm (Grassberger and Procaccia, 1983) is employed. The algorithm uses the concept of phase-space reconstruction for representing the dynamics of the system from an available time series. Using a (single-variable) time series $X_i$, where $i$=1, 2, ..., $N$, the (multi-dimensional) phase-space can be reconstructed using the method of delays, according to (Takens, 1981):

$$\boldsymbol{Y}_j=X_j,X_{j+\tau},X_{j+2\tau},...,X_{j+(m-1)\tau}), \tag{7}$$

where $j$=1, 2, ...., $N$-($m$-1) $\tau/\Delta t$; $m$ is the dimension of the vector $\boldsymbol{Y}_j$, also called the embedding dimension; $\tau$ is a delay time, and $\Delta t$ is the sampling time. For an $m$-dimensional phase-space, the correlation function $C(r)$ is given by

$$C\,(r)=\lim_{N\to\infty}\frac{2}{N\,(N-1)}\sum_{\substack{i,j\\(1\le i<j\le N)}}H\left(r-\left|\boldsymbol{Y}_i-\boldsymbol{Y}_j\right|\right), \tag{8}$$

where $H$ is the Heaviside step function, with $H(u)$=1 for $u$>0, and $H(u)$=0 for $u\le 0$, where $u$=$r-|\boldsymbol{Y}_i-\boldsymbol{Y}_j|$, $r$ is the radius of sphere centered on $\boldsymbol{Y}_i$ or $\boldsymbol{Y}_j$. If the time series is characterized by an attractor, then the correlation function $C(r)$ and the radius $r$ are related according to:

$$\underset{\substack{r\to 0\\N\to\infty}}{C(r)}\ \approx\ \alpha\,r^{\nu}, \tag{9}$$

where $\alpha$ is a constant and $\nu$ is the correlation exponent or the slope of the Log $C(r)$ versus Log $r$ plot. The slope is generally estimated by a least square fit of a straight line over a certain range of $r$. The presence/absence of determinism in the series can be identified using the correlation exponent ($\nu$) versus embedding dimension ($m$) plot. If $\nu$ saturates after a certain $m$ and the saturation value is low, then the system is generally considered to exhibit low-dimensional deterministic behavior. The saturation value of $\nu$ is defined as the correlation dimension ($d$) of the attractor. On the other hand, if $\nu$ increases without bound with increase in $m$, the system under investigation is generally considered as stochastic.

## 4 Analyses, results and discussion

### 4.1 Study area

A simplified representation of the upper alluvial aquifer of the western San Joaquin Valley is used here as a reference system for studying regional solute transport in heterogeneous aquifers. In the western San Joaquin Valley, three major hydrogeologic units are recognized: an upper semi-confined aquifer of approximately 100 m–200 m thickness, a middle confining layer with a thickness of several tens of meters (referred to as the "Corcoran Clay"), and a lower confined aquifer (several hundred meters thick). This work focuses on the upper, semi-confined aquifer. The system is bounded by the consolidated, low permeable rocks of the Coast Range complex to the west and by the Corcoran Clay below, a laterally extensive lacustrine deposit with low hydraulic conductivity. The groundwater flow system is further bound by the Thalweg of the San Joaquin Valley to the east, represented by the San Joaquin River, which is a discharge boundary for both the western and the eastern San Joaquin Valley groundwater flow systems. To the north and south, the study area is approximately bounded parallel to historic regional flow lines. The geological material in the upper semi-confined aquifer consists of Coast Range alluvium in the western region and Sierran sand with shallow flood-basin overburden near the eastern edge of the region. The drilling log data indicate that the aquifer is composed of alternative layers of coarse and fine textured material (Belitz and Phillips, 1995). Some well logs suggest that additional intermediate textured materials are present albeit poorly defined. For this study, we assume that the alluvial depositional system can be described as either a binary facies system (fine and coarse textured) or, alternatively, a triple facies system (fine, intermediate, and coarse textured).

Regional groundwater salinity transport is of prime importance in this aquifer as a result of a fundamental shift in groundwater dynamics that has occurred over the past century. Saline groundwater with dissolved solids concentrations from 983 to 35 000 mg/L has historically been found near the shallow water table within salt-enriched shallow alluvial deposits derived from marine sedimentary source rocks. Allochthone salinity generally decreases with depth. Historically, groundwater flow bypassed much of the shallow salinity at depth as mountain front recharge on the western edge was transferred laterally through the deeper portions of the aquifer system to the Thalweg at the eastern edge, where it discharged into the San Joaquin River. In the early to mid 20$^{\text{th}}$ century, extensive groundwater development began and large water import projects were constructed with

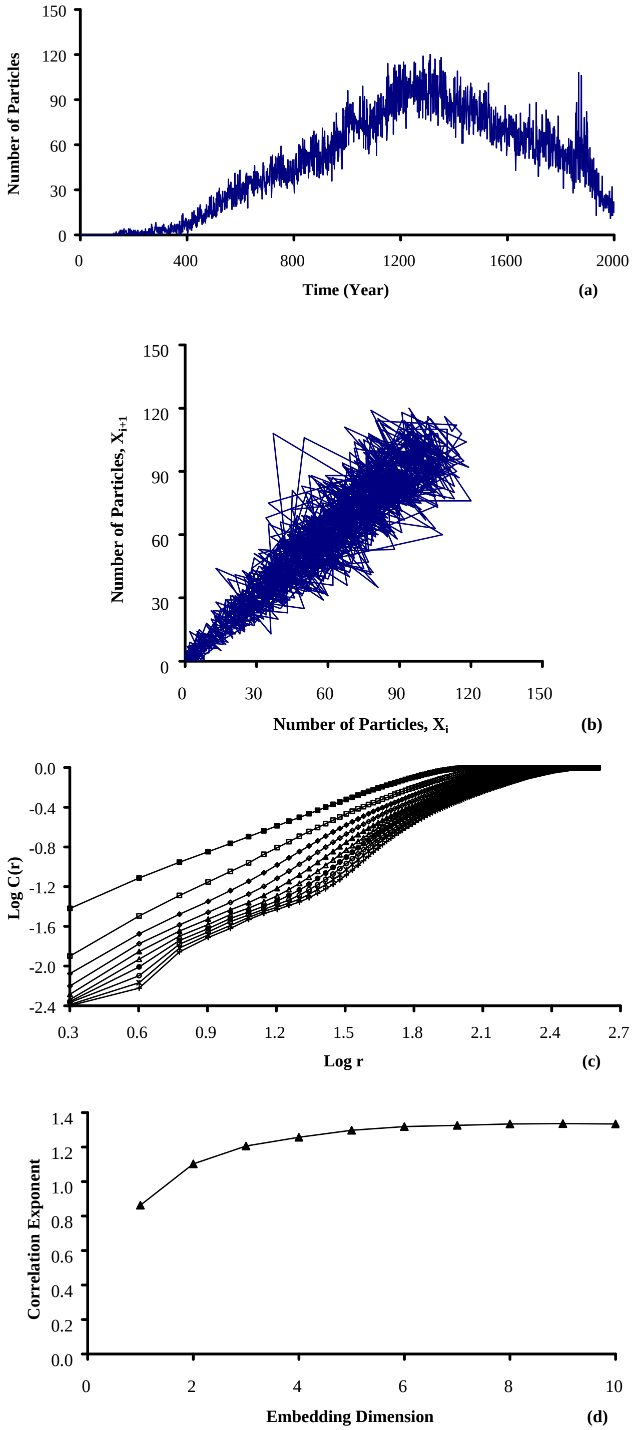


**Fig. 1.** Correlation dimension analysis of solute transport process in two facies medium (sand 20%, clay 80%) with anisotropy condition 2:1 and 50:1: **(a)** time series plot; **(b)** phase-space diagram; **(c)** Log $C(r)$ versus Log $r$ plot; and **(d)** correlation exponent vs. embedding dimension.

the introduction of intensive agricultural production. As a result, diffuse recharge from irrigation water became a large source of aquifer recharge, while significant regionally distributed pumping occurred at depth within and below the semi-confined aquifer. As a result, regional groundwater flow dynamics are now dominated by vertically downward net flux. The downward flux has mobilized shallow salinity and is transporting salts perpendicular to the dominant alluvial layering to lower portions of the aquifer. According to Belitz and Phillips (1995), the regional downward flux is on the order of 0.3 m/yr. However, the presence of interconnected coarse-textured sand and gravel facies within the semi-confined aquifer and the Corcoran Clay could significantly accelerate the migration of highly saline groundwater to the deep semi-confined and confined aquifer zones and potentially lead to the early degradation of water quality in the production zone.

### 4.2 TP/MC, MODFLOW and RWHet model specifications

Borehole data and soils maps are used to determine the appropriate TP/MC models (Weissmann et al., 1999). For the analysis here, the semi-confined upper aquifer is conceptually represented by a simple rectangular, three-dimensional 111×111×111 grid structure. To avoid numerical edge effects associated with the TProGS simulation (Steve Carle, personal communications), five layers from each of the edges are eliminated after the random field generation. The final structure of the medium for flow and transport modeling contains 101×101×101 (=1 030 301) cells.

Using the TP/MC model, aquifer heterogeneity realizations are generated for varying plausible combinations of the four hydrostratigraphic parameters, given the limited amount of field data (sensitivity analysis). These include: (1) two alternate simplified facies models: two (sand and clay) vs. three (sand, clay, and loam) explicit facies; (2) 30 combinations of proportions in two facies (sand from 15% to 60% and clay forming the remainder) and one combination of proportions in three facies (i.e. sand 21.26%, clay 53.28%, and loam 25.46%); (3) three sets of mean length ratios (ratios of dip to strike and dip to vertical facies mean length are 2:1 and 300:1, 5:1 and 300:1, and 2:1 and 50:1); and (4) three combinations of juxtapositional tendencies or entropies: maximum entropy or random juxtaposition of facies, intermediate entropy, and low entropy or highly structured order of facies, e.g. loam is almost always located above sand and below clay (fining upward), not vice versa. For further details on this sensitivity analysis, the reader is referred to the study by Zhang et al. (2004)[1].

For the flow simulations, boundary conditions include a uniform constant head $H_1$ at the top and a uniform constant head $H_2$ at the bottom, such that $H_1$–$H_2$=10.7 m. No flow is specified at all vertical sides of the regional model domain. The model aquifer is 123.1 m deep with grid block thickness fixed at 1.2 m. In all simulations, grid discretization is equal to $^1/_4$ of the mean length in any principal direction. Hence, in the dip and strike directions, horizontal discretization varies

[1]Zhang, H., Harter, T., and Sivakumar, B.: Transition probability/Markov chain approach: Sensitivity analysis of nonpoint source solute transport normal to alluvial facies bedding, Water Resour. Res., submitted, 2004.

with mean length ratio. In the dip direction, grid size ranges from 61.0 m to 365.8 m. In the strike direction, grid discretization ranges from 30.5 m to 182.9 m. The resulting lateral extent of the simulated aquifer varies from 3.1 to 18.5 km and from 6.2 to 36.9 km for the dip and strike directions, respectively. The simulated, rectangular simulation domain is considered a simplified but conceptually representative subsection of the approximately 30–40 km (east-west) by more than 100 km (north-south) large western San Joaquin Valley system.

Hydraulic conductivity ($K$) is assigned to each cell corresponding to the simulated hydrofacies from each geostatistical realization scenario. Values of hydraulic conductivities of (each) hydrofacies correspond to those for sand and fine-grained facies in the calibrated model of Belitz and Phillips (1995): 9.5 m/d for sand, 0.0012 m/d for clay. A low intermediate value of 0.012 m/d is assumed for loam (muddy sand).

To compute travel time, a single pulse of particles (representing salinity) is injected at the top: Ten particles are uniformly placed in every cell in the second layer from the top (a constant head is set for the top layer). The regional breakthrough curve (BTC) is monitored by recording the number of particles arriving at the bottom layer. Local dispersion and molecular diffusion are ignored such that the BTCs represent only variations in travel time due to local variability in advection velocity through the simulation domain. Effective porosity is assumed uniform at 30%. After ignoring local dispersion and diffusion, the maximum travel time is bounded at approximately two millennia.

### 4.3 Data, analyses and results

#### 4.3.1 Number of facies

In the sensitivity analysis of solute transport to number of facies, two types of facies models are considered: a simple two-facies model that effectively corresponds to an indicator random field generated from a cutoff in a Gaussian random field; and a three facies model representing three major hydrofacies in alluvial systems: sand and gravel facies, muddy sand facies, and mud facies. Figure 1a, for instance, shows the breakthrough curve for salt transport (i.e. time series of particle arrival) in two facies (sand 20%, clay 80%), while the breakthrough curve for the three facies medium is shown in Fig. 2a. Both these curves correspond to mean length anisotropy ratios 2:1 and 50:1, and field entropy in three facies.

Figures 1b and 2b show, respectively, the phase-space diagrams of these time series, reconstructed according to Eq. (7). The figures correspond to phase-space reconstruction in two dimensions (i.e. $m$=2), with delay time $\tau$=1 year (a typical sampling interval for ambient groundwater monitoring), i.e. the projection of the attractor on the plane ($X_i$, $X_{i+1}$). As may be seen, the projection yields reasonably well-defined attractors for both the series, suggesting the possibility of deterministic dynamics. Figures 1c and 2c present

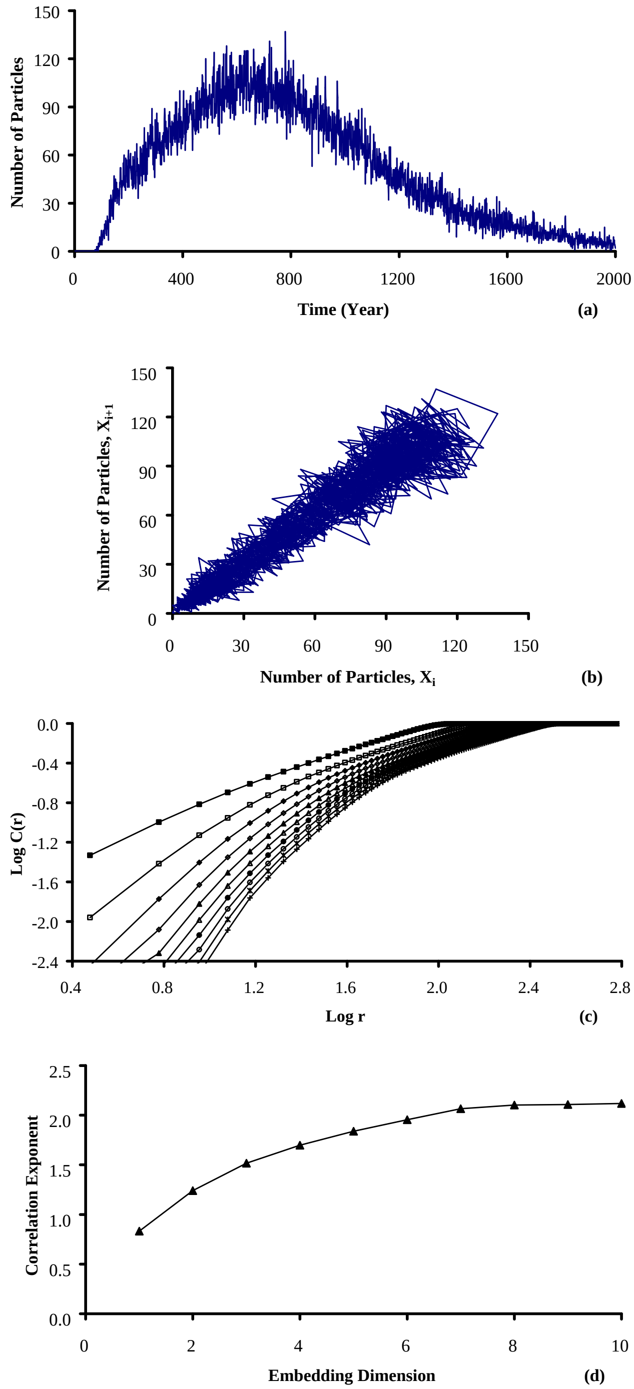


**Fig. 2.** Correlation dimension analysis of solute transport process in three facies medium (sand 21.26%, clay 53.28%, loam 25.46%) with anisotropy condition 2:1 and 50:1 and field entropy: **(a)** time series plot; **(b)** phase-space diagram; **(c)** Log $C(r)$ versus Log $r$ plot; and **(d)** correlation exponent vs. embedding dimension.

the relationship between correlation integral ($C(r)$) and radius ($r$) for embedding dimensions ($m$) from 1 to 10 for these two series, respectively, and Figs. 1d and 2d present the relationship between correlation exponent values and embedding dimension values. For both the series, the correlation

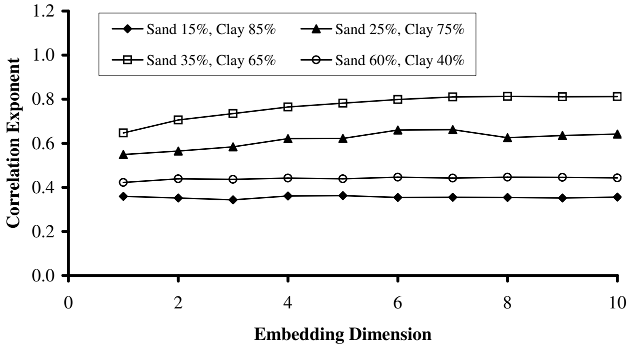


**Fig. 3.** Effect of volume proportions on solute transport behavior in two facies medium (with anisotropy condition 2:1 and 300:1): sand 15%, clay 85%; sand 25%, clay 75%; sand 35%, clay 65%; and sand 60%, clay 40%.

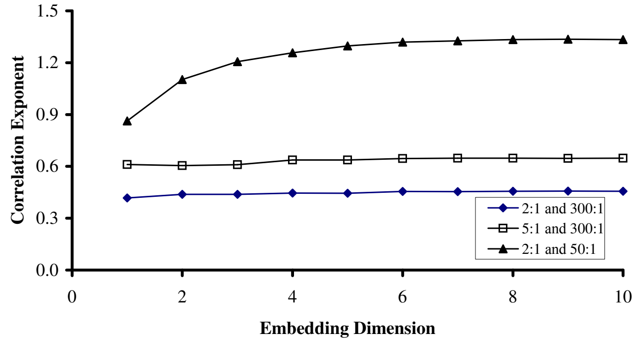


**Fig. 4.** Sensitivity of dynamic behavior of solute transport process to anisotropy conditions in two facies medium: sand 20%, clay 80%.

exponent value increases with the embedding dimension up to a certain point, and saturates beyond that point. The saturation values (i.e. correlation dimensions) are as low as 1.33 and 2.12 for these series, respectively, indicating that the dynamical behaviors of solute transport processes may be low-dimensional deterministic in nature. As the nearest integer above the correlation dimension provides the number of variables dominantly governing the dynamics, the above correlation dimensions suggest that the solute transport dynamics in the two and three facies media are dominantly governed by as few as 2 and 3 variables, respectively. These results also indicate that the complexity of the solute transport process in the three facies medium is higher than that in the two facies medium (for the above proportions, anisotropy and entropy conditions; see below for further details).

### 4.3.2 Volume proportions of facies

The volume proportions are varied only in the two facies medium, and a total of 30 combinations (sand varying from 15% to 60%, while clay forming the remainder) are considered. Figure 3, for instance, presents the dimension results for particle arrival time series simulated with four different sand proportions (15%, 25%, 35%, and 60%). The four series are simulated for strongly layered conditions with anisotropy ratios of 2:1 (dip:strike) and 300:1 (dip:vertical). Finite and low correlation dimensions are observed for all the cases, suggesting presence of deterministic dynamics. Dimensions of 0.35, 0.62, 0.81, and 0.44 for the four series indicate that the solute transport dynamics are dominantly governed by only one variable. However, the complexity of the process slightly increases with an increase in sand proportion up to a certain point and then decreases with further increase in sand (similar results are observed also for the other two anisotropy conditions). This is understandable, since only certain mechanisms may have dominant influence on the solute transport process in the presence of either very small or very large sand proportions, even though the connectivities may have opposite characteristics. The transport process becomes more heterogeneous when sand and clay proportions approach each other, as there may be additional mechanisms due to (significant) influence of both sand and clay. This is consistent with the fact that, at a given hydraulic conductivity contrast, the highest variance of the binary aquifer system is obtained when the two facies are present in equal proportions. It appears that there is a correlation between the dimension parameter and system variance.

In spite of this explanation, one aspect that may be surprising is that the solute transport process is dominantly governed by only one variable, irrespective of the sand proportion. The next section investigates, to which degree the mean length anisotropy ratios may modify these findings.

### 4.3.3 Mean length anisotropy

The analysis is performed for all three anisotropy conditions (2:1 and 300:1, 5:1 and 300:1, and 2:1 and 50:1) for each of the 30 combinations (sand proportions) in the two facies medium and each of the 3 combinations (juxtapositional tendencies) in the three facies medium. Figure 4, for instance, presents the correlation dimension results obtained for the three anisotropy conditions in the two facies medium with sand proportion equal to 20% (clay 80%). The correlation dimension values are found to be as low as 0.46, 0.64, and 1.33, respectively, suggesting the presence of deterministic dynamics in the transport process. The extent of difference in the dimension results between the three anisotropy conditions indicates that a change in ratio of dip to vertical mean length (from 2:1 and 300:1 to 2:1 and 50:1) has much more influence on solute transport than a change in ratio of dip to strike mean length (from 2:1 and 300:1 to 5:1 and 300:1). This is due to the vertical mean flow in the system. Similar results are observed also for other sand proportions in the two facies medium and for different entropy conditions in the three facies medium (figures not shown), but the dynamics tend to become much more complex with anisotropy condition 2:1 and 50:1 for certain proportions and entropies. This is consistent with the fact the the velocity field is more complex in the less stratified system (lower anisotropy). The significance lies in the fact that the dimension parameter appears sensitive to these changes in the velocity field complexity within the aquifer without being directly informed about the velocity.

#### 4.3.4 Juxtapositional preferences

Entropy (degree of order) in the facies structure plays an important role in connectivity (high entropy refers to less order). In classical stochastic theory, the aquifer medium is generally considered to exhibit high (or maximum) entropy, as a Gaussian random field is assumed for hydraulic conductivity. In the TP/MC approach, however, different levels of entropy may be considered to represent the medium, which are indicated by "juxtapositional tendencies" of the bedding sequences. Therefore, the TP/MC approach has the ability to represent different possibilities of order of facies, anywhere between determinism and randomness. This aspect is crucial from a practical point of view, since natural aquifers possess different levels of heterogeneity.

In the sensitivity analysis, three different entropy conditions in the three facies medium are considered: maximum, field, and low entropy. Figure 5, for instance, presents the correlation dimension results for the these entropy conditions when the anisotropy condition is 5:1 and 300:1. The solute transport process in these cases exhibit low correlation dimensions of 0.95, 1.02, and 1.11, respectively, suggesting the presence of deterministic dynamic behavior in the solute transport process, governed dominantly by as few as 2 variables. The results also indicate increasing complexity of the solute transport process with an increasing order of facies in the aquifer medium (similar results are also observed for solute transport process simulated with the other two anisotropy conditions, i.e. 2:1 and 300:1 and 2:1 and 50:1, figures not presented). The effect is, again, related to the complexity of the velocity field, which can be (and in this example is) larger in media with a higher ordered structure than in media with a purely random conductivity distribution.

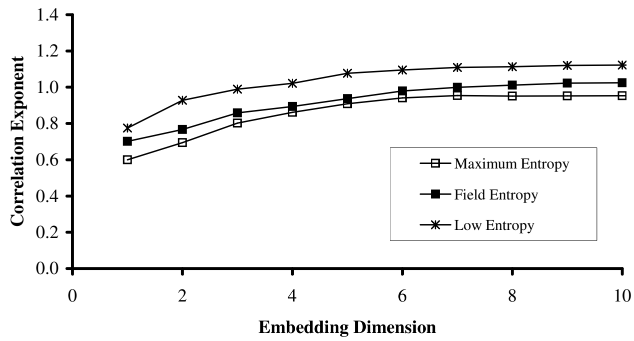


**Fig. 5.** Effect of entropy on solute transport behavior in three facies medium (sand 21.26%, clay 53.28%, loam 25.46%) with anisotropy condition 5:1 and 300:1.

## 5 Conclusions and potential for further research

The present study investigated the possible nonlinear deterministic nature of solute transport process in a heterogeneous aquifer medium. Employing a dimension concept to time series of particle transport (i.e. an inverse approach), the study presented preliminary evidence to nonlinear deterministic dynamics in the transport process, even though more complex behaviors cannot be excluded for certain hydrostratigraphic conditions. Sensitivity analysis of solute transport behavior to hydrostratigraphic parameters revealed not only the importance of such parameters in representing aquifer heterogeneity but – most importantly – the ability of the dimension concept in representing the (extent of) complexity of the dynamics, at least on a comparative basis.

In spite of its preliminary nature, the present investigation provides important clues to the use of nonlinear deterministic techniques as a viable alternative to study subsurface problems. Verification and confirmation of the present results through use of other nonlinear deterministic techniques are necessary to be more assertive of such a notion (see Sivakumar, 2000, 2004; Sivakumar et al. 2002b for details). Also, as the solute transport scenarios simulated and investigated in this study are only a limited case of the possible ones, the reliability of the present results needs to be assessed by studying other transport scenarios. Supplementing and complementing the present inverse approach results using the "physics" of solute transport process remains an important problem to be resolved. Arguably, the most crucial task is to find ways to extend the (present) one-dimensional analysis technique(s) to three-dimensional fields, a situation that is much more prevalent in subsurface flow and transport problems. Studies in these directions are underway, details of which will be reported elsewhere.

*Acknowledgements.* Funding for this work was provided by the Collaborative UC/Los Alamos Research program (University of California Directed Research Development) and by the University of California Salinity/Drainage Program. The authors would like to thank D. Zhang, C. Puente, and N. Ruud for useful discussions. The authors would also like to thank M. Giudici and an anonymous reviewer of their constructive comments on an earlier version of this manuscript.

Edited by: R. Berndtsson
Reviewed by: M. Giudici and another referee

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